Nanomat_oving_8

November 7, 2024

[ ]:
```python
import matplotlib.pyplot as plt
import numpy as np

pCO = np.array([13.3, 26.7, 40.0, 53.3, 66.7, 80.0, 93.3]) # Pressure of CO␣
 ↪[kPa]
vCO = np.array([10.3, 19.3, 27.3, 34.1, 40.0, 45.5, 48.0]) # Volume of CO [cm^3]

fig, axs = plt.subplots()
axs.scatter(pCO,pCO/vCO, marker='x', label='Datapoints') # Scatter plot of␣
 ↪pressure vs pressure/volume ratio

# Perform linear regression to fit a line through the data points
coeffs = np.polyfit(pCO, pCO / vCO, 1)

# Calculate the x values of the regression line
pCO_reg = np.linspace(pCO.min()*0.95, pCO.max()*1.05, 100)

# Plot the linear regression line
axs.plot(pCO_reg, pCO_reg*coeffs[0]+coeffs[1], label='Linear regression',␣
 ↪color='red')

# Add a legend to the plot
fig.legend(loc='upper left', bbox_to_anchor=(0.12, 0.885))

# Set the labels and title of the plot
axs.set_ylabel(r'$p/V\ [kPa/cm^3]$')
axs.set_xlabel(r'p [kPa]')
axs.set_title('Gas adsorption measurements on carbon black.')

# Print the slope of the linear regression line
print(f"Slope of regression line (1/v_mono): {coeffs[0]:.2e} [m^3/kPa]")

### Find the number of CO molecules ###
T = 293 # Temperature [K]
p_atmosphere = 101325 # Pressure [Pa]
R = 8.314 # Gas constant [J mol^-1 K^-1]
N_A = 6.022e23 # Avogadro constant [mol^-1]
```

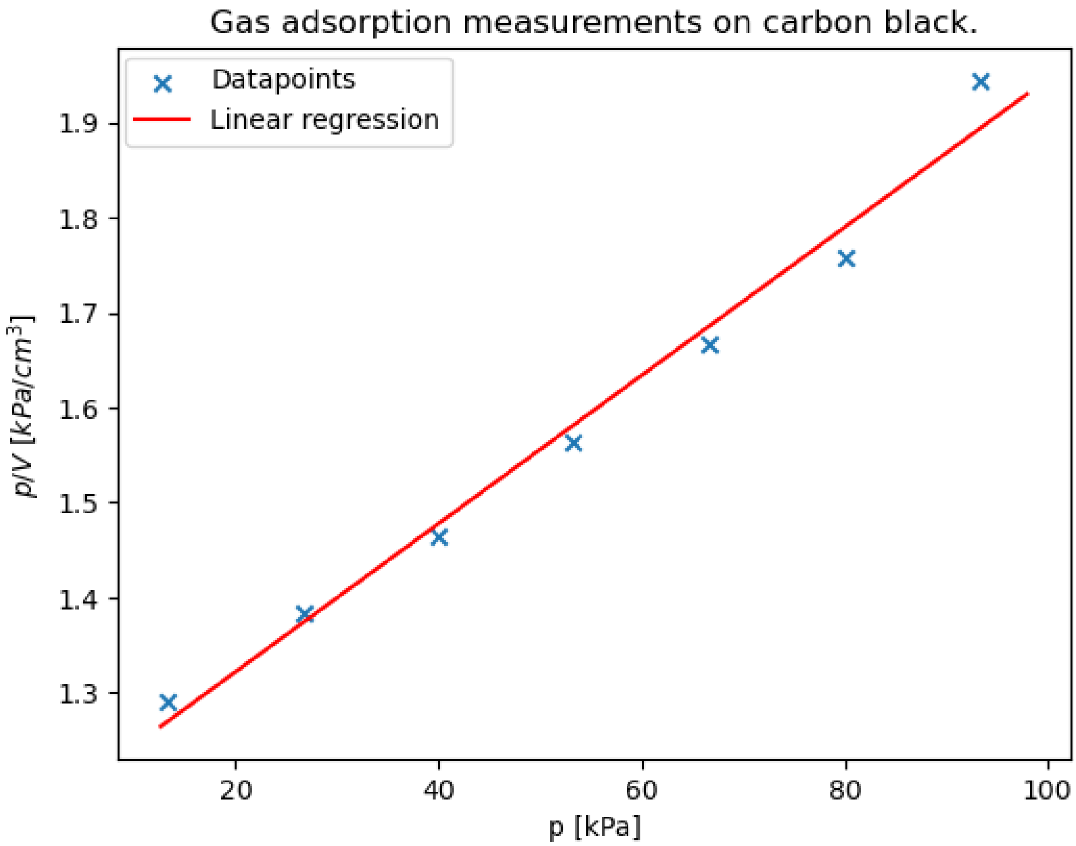
```python
v_mono = (coeffs[0]**-1)*1e-6 # Volume of a single CO molecule [m^3]
n_CO = p_atmosphere*v_mono/(R*T) # Number of CO molecules: Ideal gas law pV =
 ↪nRT
print(f"Number of CO molecules: {n_CO:.2e} [mol]")


### Calculate the specific surface area ###
Area_CO = 0.16*1e-18 # [m^2] - Specific occupiued surface area of a CO molecule
Area_tot = n_CO * Area_CO * N_A # [m^2] - Total occupiued surface area of the
 ↪carbon black
print(f"Total surface area: {Area_tot:.2e} [m^2]")

### Adjust for mass ###     CB is Carbon Black
mass_CB = 9.659 # Mass of sample [g]
density_CB =  2.1*1e6 # Density of sample [g/m^3]
spesific_surface_area = Area_tot/mass_CB # [m^2/g]
print(f"Spesific surface area: {spesific_surface_area:.2e} [m^2/g]")

### Find the radius of the carbon black ###
radius_CB = (3/(spesific_surface_area*density_CB)) # [m]
print(f"Radius of carbon black: {radius_CB*1e9:.1f} [nm]")
print(f"Diameter of carbon black: {2*radius_CB*1e9:.1f} [nm]")
```

```
Slope of regression line (1/v_mono): 7.79e-03 [m^3/kPa]
Number of CO molecules: 5.34e-03 [mol]
Total surface area: 5.14e+02 [m^2]
Spesific surface area: 5.32e+01 [m^2/g]
Radius of carbon black: 26.8 [nm]
Diameter of carbon black: 53.7 [nm]
```


Gas adsorption measurements on carbon black.
Datapoints
Linear regression
1.9
1.8
1.7
1.6
1.5
1.4
1.3
p/V [kPa/cm^3]
20
40
60
80
100
p [kPa]